Innovative Reviews in Engineering and Science, ISSN: 3048-8745 Vol. 3, No. 2, 2026 (pp. 117-124)
RESEARCH ARTICLE
ECEJOURNALS.IN

Advances in Functional Nanomaterials for Energy Storage and Conversion: A Comprehensive Review of Mechanisms, Materials, and Applications

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KEYWORDS:
Functional nanomaterials,
Energy storage,
Energy conversion,
Batteries,
Supercapacitors,
Electrocatalysts,
Photocatalysis,
MOFs,
Perovskites,
Nanotechnology

ARTICLE HISTORY:
Submitted : 18.02.2026
Revised : 20.03.2026
Accepted : 10.05.2026

https://doi.org/10.31838/INES/03.02.13

Abstract

Moving towards durable and efficient energy regimes requires new materials that will offer high performance energy storage and conversion. The review highlights the latest developments in functional nanomaterials and elaborates on their structural composition, synthesis methodologies as well as their potential applications in the area of batteries, supercapacitors, fuel cells and photocatalytic/electrocatalytic systems. The key task is to investigate the role of nanomaterials (i.e. metal oxides, carbon-based materials (e.g. graphene, CNTs), metalorganic frameworks (MOFs), perovskites, and transition metal dichalcogenides (TMDs)) in the improvement of the device performance due to its morphology engineering, quantum confinement effects, and interfacial design. The approaches to the synthesis (e.g., sol-gel, hydrothermal, CVD, electrospinning) are evaluated comparatively to note the possibilities of scaling it and its cost and environmental impact. Critical discussion on key performance indices such as energy density, power density, cyclic stability and charge transport dynamics are discussed. Limits to modern technologies which are structural degradation, poor cycle life, and interfacial charge recombination are also identified in the review and addressed by heterostructure engineering and hybrid nanocomposites. Combining the knowledge of the recent experimental and theoretical works aimed at smart hybrid nanostructures and green synthesis, the article proposes the future perspectives of green synthesis, smart hybrid systems, and materials discovery with the guidance of AI. This review was created with the intention of forming the basis on which other researchers and engineers work on new generations of multifunctional nanom.

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How to cite this article: Re-Ann C, Abdullah D. Advances in Functional Nanomaterials for Energy Storage and Conversion: A Comprehensive Review of Mechanisms, Materials, and Applications. Innovative Reviews in Engineering and Science, Vol. 3, No. 2, 2026 (pp. 117-124).

Introduction

The increase in world energy needs, as well as economic and environmental considerations and dwindling non-renewable fuel sources has boosted the transition into sustainable and renewable systems of energy provision. An important facilitator of this transition is in the feasibility of creating advanced energy materials that are both highly efficient, friendly to the environment and multifunctional. Of these, functional nanomaterials have drawn great deal of fascination particularly because of their unique physicochemical characteristic of its huge surface area, ability to enhance electronic/ionic conduction and tailorable band structure since the characteristic of quantum confinement plays a key role.[1, 2] Nanostructured materials are the key materials to various energy storage and conversion mechanisms such as lithium/sodium-ion batteries, supercapacitors, fuel cells, thermoelectrics, and photocatalytic/ electro catalytic platforms.[3] They provide strategic route to enhance energy density, power output and device stability, in part due to their capability to host rapid redox reactions, a wide variety of active sites, and interfacial engineering. Although recent progress was quite fast, the current literature tends to concentrate on either individual material groups or selected applications, not providing a unified, cross-platform investigation, linking material structure property connections with performance functions.[4] Additionally, there is an issue concerning scalability of processes and stability during operation and on the environment framed issues concerning soundness of nanomaterial synthesis processes.[5] There is an increasing importance of the need to apply sustainable, scalable and intelligent design strategies to bridge the gap between a lab-scale innovation and commercial deployment.

The review intends to give an integrative and exhaustive overview of recent advances on functional nanomaterials to energy storage and conversion. It identifies important material systems, including metal oxides, carbon-based nanostructures, metal organic frameworks (MOFs), perovskites and transition metal dichalcogenides (TMDs). In addition, it explores the synthesis strategies, carrier transportation, integration of devices and future developments like Artificial intelligence-driven material discovery and eco-friendly manufacturing.

Related Work and Research Background

During the last decade, extraordinary progress in development of functional nanomaterials applicable to energy-related technologies is observed. These initiatives go into the breakthroughs of nanomaterial synthesis, functionalization and use in electrochemical and photonic devices. Improvement of energy density, charge discharge performance, stability and environmental compatibilities of energy storage and conversion systems has been the main priority.

Nanomaterials in Electrochemical Energy Storage

Nanostructured materials also profoundly augment the work of batteries and supercapacitors since they do allow extensive surface areas, reduce ion diffusion distances, and also enhance electrical conductivity. Zhang et al.[6] considered carbon-based nanomaterials in lithium-ion battery, with particular attention paid to the discussed role of surface area engineering, heteroatom doping, and interfacial modification in enhancing reversible capacity and cyclic life. To produce hybrid supercapacitor cells Wang et al.[7] have conducted another study in which the high pseudocapacitive material was hierarchical oxide of metals like MnO 2 and NiCo 2 O 4, which were capable of producing swift redox kinetics and superior energy densities in hybrid supercapacitor cells.

Nanostructures for Photocatalysis and Solar Fuel Generation

Clean fuel production is attracting photocatalytic water splitting and energy-efficient CO 2 reduction via solar energy. Perovskite nanomaterials and graphitic carbon nitride (g-C3N4) show tunability and optimal absorption in the visible light, thus posses superior qualities in harnessing solar energy. Chen et al. [3] have proposed two heterostructure engineering methods which include Z-scheme and Schottky junction in order to maximize charge separation during photo generation. Also, Singh et al.[8] discussed the structural flexibility of MOFs in supporting and carrying out CO 2 photoreduction at ambient conditions as catalysts and scaffolds.

Functional Nanomaterials for Fuel Cell and Electro-catalytic Applications

The literature currently holds platinum-based materials as the standard one in oxygen reduction reactions (ORR) in fuel cell systems, although its cost and low availability do not support massive implementation. Other electrocatalysts that have been studied recently include transition metal dichalcogenides (TMDs), heteroatom-doped carbon nanostructures (e.g., N, S co-doped graphene). Li et al.[9] proved these nano-structures are catalytically active enough at reduced cost and increased stability as compared to their doped counterparts. Zhao et al.[10] also studied the possibility of using MOF derived carbon materials due to their highly adjustable porosity and surface chemistry and maximizing their performance as electrocatalysts in systems.

Challenges in Scalability and Environmental Impact

Although with encouraging laboratory findings, majority of the high-performing nanomaterials are restricted by scalability, long-term stability and environmental sustainability. Kumar et al.[11] pointed out that most of the processes of the synthesis of nanomaterials use hazardous liquids and energy-expensive stages. In response to this, there is a push towards the green synthesis methods, life cycle analysis (LCA), and real operating conditions in-situ degradation studies.

Research Gaps

Although substantial progress has already been made, there is the lack of general review and current research on one hand owing to domain specificity (e.g. only on a material system, such as carbon nanostructures or MOFs) and a domain of application (e.g. only lithium-ion batteries). The synergistic nature of multi-component nanomaterials and cross-platform strategy remains a gaping area of knowledge. Moreover, the systematic comparisons of synthesis paths, structure-property relationships and integration problems in devices are rare.[20] This review aims to provides ways of closing such gaps by producing a general overview and comparative analysis of various functional nanomaterials and applications thereof in electrochemical, photocatalytic and electrocatalytic energy platforms.

Classification of Functional Nanomaterials

The functional nanomaterials used in the energy storage and conversion systems may be categorized into broad groups on the bases of composition, structure, and physicochemical properties. The respective classes of materials have different benefits in terms of customization of electronic, ionic and catalytic performance required in high-performance energy devices. The below mentioned subsections segregate the most notable nanomaterial systems developed in the ongoing energy researches.

Metal Oxides (e.g., TiO_2, MnO_2, Fe_3O_4)

Metal oxides are the most popular nanomaterials given their rich redox chemistry, low cost and tunability of structure. In particular TiO 2 and MnO 2 exhibit high surface area, stable crystalline structures, and are reversibly permeable to charge, so that they make suitable lithium-ion batteries and pseudo-capacitors.[12] They can be engineerally perfected to be in the form of nanowires, nanosheets, or mesoporous frameworks to maximize ion diffusion kinetics and contact area of the electrode to the electrolyte. These types of structures and related energy uses are shown in Figure 1: Structural Forms, Properties, and Energy Applications of Metal Oxide Nanomaterials (e.g., TiO 2 , MnO 2 , Fe 3 O 4). Such difficulties with low intrinsic electrical conductivity, however, can require composite materials be made, generally with conductive agents (such as carbon nanotubes or graphene), to improve overall electric behavior.[19]

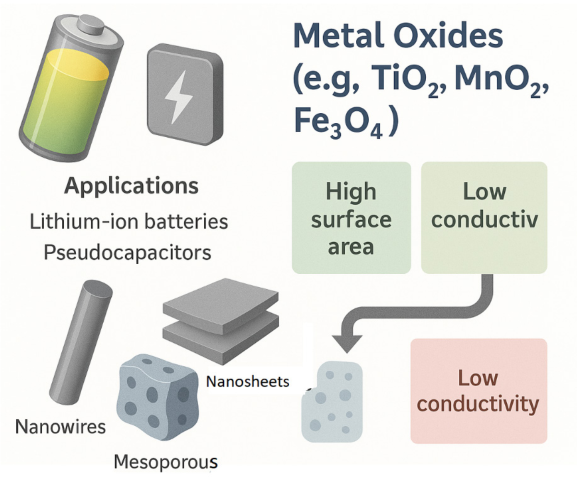

Fig. 1: Structural Forms, Properties, and Energy Applications of Metal Oxide Nanomaterials (e.g., TiO_2, MnO_2, Fe_3O_4)

Carbon-Based Nanomaterials

Carbon nanostructures innate good electrons conduction, mechanical flexibility and electrochemical stability, such as graphene, carbon nanotubes (CNTs), and carbon dots. These characteristics are what render them essential in use in supercapacitors, catalytic support of electrocatalysts as well as electrodes constructed of composite materials.[13] The 2-dimensional structure of graphene offers large charge carrier mobility and defect-tolerance and CNTs offer high aspect ratio conduction channels suitable to fast transport of electrons. Hybrid materials give rise to this synergy and result in increased specific capacitance and electrode stability in a combination of carbon structures with other functional elements (e.g., metal oxides or TMDs). The energy relevant properties of the carbon-based nanomaterials can be found in the Figure 2: Structures, Properties, and Energy Applications of Carbon-Based Nanomaterials (Graphene, CNTs, and Carbon Dots).[21]

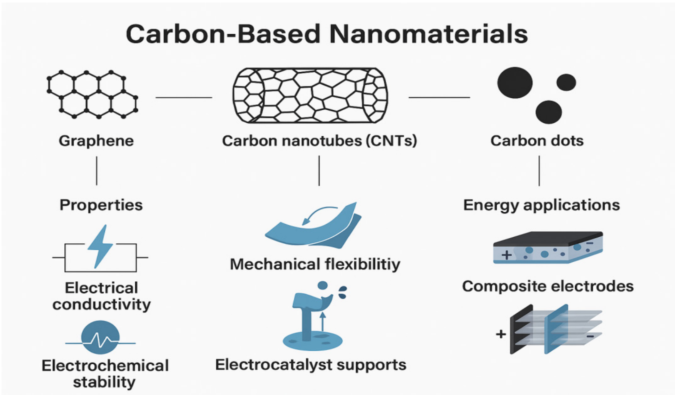

Fig. 2: Structures, Properties, and Energy Applications of Carbon-Based Nanomaterials (Graphene, CNTs, and Carbon Dots)

Metal-Organic Frameworks (MOFs) and Derived Nano-structures

MOFs are crystalline hybrid materials, comprising metals nodes coordinated to organic ligands, producing high porosity and huge surface areas, with portable pore chemistry. These characteristics earn them the best repeat candidates under gas storage, heterogeneous catalysis and electrical applications.[14] The intrinsic structure of MOFs also allows the conversion to porous carbon through conversion into heteroatom-doped porous carbon frameworks through pyrolysis with retention of high surface activity and charge transport (illustration in Figure 3: Properties, Structure, and Energy Applications of MetalOrganic Frameworks (MOFs) and Their Pyrolyzed Derivatives). These derivatives show great electrocatalytic activity towards oxygen

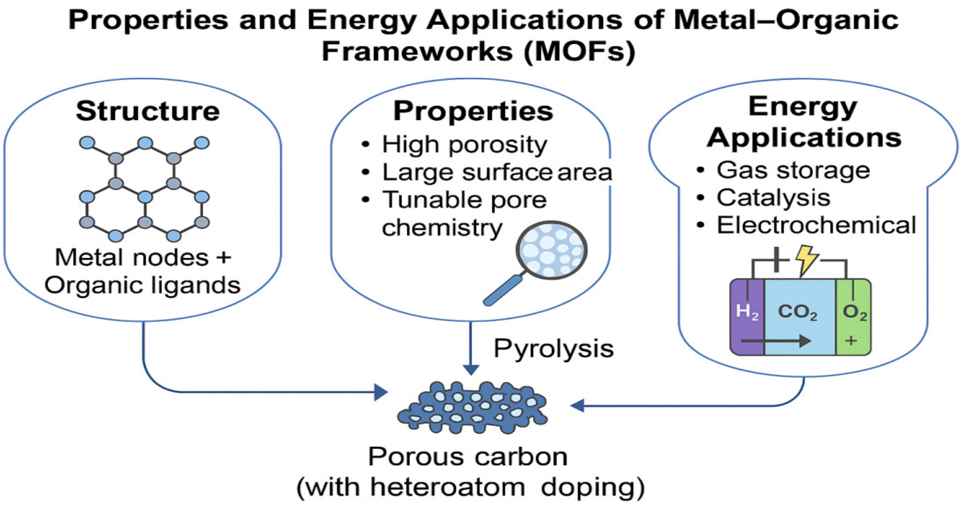

Fig. 3: Properties, Structure, and Energy Applications of Metal-Organic Frameworks (MOFs) and Their Pyrolyzed Derivatives

reduction, CO 2 reduction and hydrogen evolution reaction. Nevertheless, issues like sensitivity to moisture and degradation of structures with long cycling operations continue to propound serious hindrances to the operational feasibility of its deployment.

Perovskite Nanomaterials

There is also the perovskite materials (ABX 3) structure with powerful light absorption capability, bandgap tunability, and long carrier diffusion length, which makes them superior photovoltaic use and photoelectrochemical water splitting.[15] These structural and optoelectronic properties have made perovskites leading material in next-generation photovoltaic and photoelectrocatalytic applications as shown in Figure 4: Crystal Structure, Key Properties, and Energy Applications of Perovskite Nanomaterials (ABX 3 -Type Compounds). Perovskites in lead, especially have transformed the field of photovoltaic research by producing power conversion efficiencies (PCEs) over a limit of 25%. Perovskites at the nanoscale give a greater level of finesse over light-harvesting and crystal quality. Nevertheless, stability issues in respect to humidity, light and thermal stress remain. Recent research trends focus on the synthesis of lead free perovskites and two dimensional (2D) perovskite heterostructures to improve durability and performance in the real life circumstances.[18]

Transition Metal Dichalcogenides (TMDs)

These materials are TMDs (e.g. MoS 2, WS 2, SnS 2) which exhibit strong in-plane covalent bonding but weak van der Waals inter-layer coupling. Their fabricated surface area, enhanced electrical conductivity, and the multiple oxidation status provide potential prospects of using them in electrocatalysis, flexible electronics, and next-generation-batteries,[16] Figure 5: Layered Structure, Properties, and Energy Applications of Transition Metal Dichalcogenides (TMDs) demonstrates that these

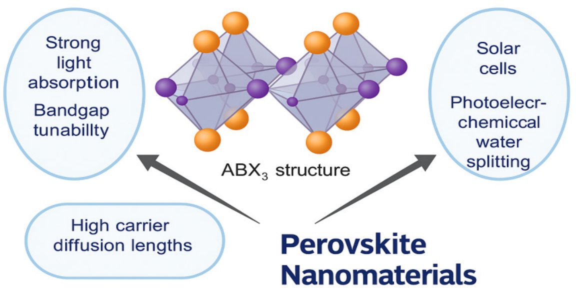

Fig. 4: Crystal Structure, Key Properties, and Energy Applications of Perovskite Nanomaterials (ABX3-Type Compounds)

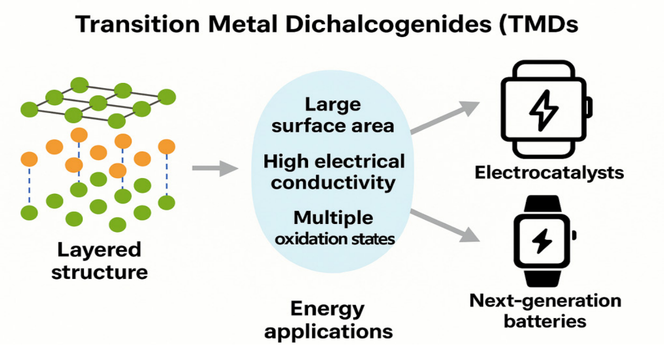

Fig. 5: Layered Structure, Properties, and Energy Applications of Transition Metal Dichalcogenides (TMDs)

materials have a variety of structural and electronic properties that make systems multifunctional in energy. The active edge sites greatly open by exposing on few-layered TMD nanosheets, especially as to the Hydrogen evolution reaction (HER) and oxygen reduction reaction (ORR). Their adoption into soft or apparel energy technologies also compliments well with the increasing need of portable, lightweight and high performing power technology solution.

Synthesis Strategies

The morphology, crystallinity, surface properties, and the overall structural integrity of a functional nanomaterial are key factors of the performance of the nanomaterial within an energy storage and conversion system and these factors are greatly affected in the synthesis phase. These physicochemical properties are largely determined by the synthesis technique chosen, thus influencing the behavior of the material on an electrochemical, photocatalytic or electrocatalytic state.[17] Figure 6: Overview of Nanomaterial Synthesis Methods shows that, in each case, a particular technique offers different degrees of shape control of the final nanostructure, which affects scale up and performance in the material end application. Four major synthesis methods, which have been widely used, such as Sol-gel, Hydrothermal, Chemical Vapor Deposition (CVD), and Electrospinning, are described in this section, where their advantages, scalability, and disadvantages are compared (Table 1 summarizes these aspects).

All these approaches have unique benefits given certain material combinations and device needs. An example is that sol-gel and electrospinning are better suited to scale up the synthesis of porous or fibrous materials to design supercapacitors or batteries but CVD is better suited to the production of high quality thin films in photovoltaic or flexible electronic devices. Hydrothermal methods continue to be the key to synthesize crystalline nanostructures with control aspect ratios, especially MOFs, TMDs and metal oxides.

Nevertheless, there are issues with the industrial scalability of laboratory-scale reproducibility. In the future, the core research aspects should be green synthesis strategies, a hybrid process, and process automation that would provide the sustainable manufacturing of nanomaterials at large scale but with stable performance characteristics.

Energy Storage Applications

The nano materials are critical in boosting the efficiency of the energy storage systems through better overall ion/electron transports, surface reactivity and stability. These materials can be designed to fit the needs of high

Table 1: Comparative Summary of Nanomaterial Synthesis Methods—Principles, Advantages, and Challenges

Method	Description	Advantages	Challenges
Sol-gel	A wet-chemical route involving the hydrolysis and condensation of metal alkoxides or salts to form a colloidal sol, which transforms into a gel and subsequently into a nanomaterial upon drying and calcination.	Precise control over composition and homogeneity; low processing temperature	Time-consuming drying and shrinkage; risk of cracking during gelation
Hydrothermal	A solution-phase synthesis carried out in sealed autoclaves at elevated temperature and pressure to promote the formation of crystalline nanostructures.	Well-defined morphology; high crystallinity; environmentally friendly (aqueous solvents)	Requires high-pressure equipment; limited throughput
Chemical Vapor Deposition (CVD)	A vapor-phase technique where precursor gases react or decompose on a heated substrate, forming high-quality thin films or nanostructures.	Produces uniform, conformal coatings; excellent purity and crystallinity	High capital cost; energy-intensive due to high operational temperatures
Electrospinning	A technique to fabricate continuous 1D nanofibers by applying a high-voltage electric field to a polymer solution or sol-gel precursor.	High surface-area-to-volume ratio; tunable fiber morphology	Requires careful polymer selection; potential for non-uniform fiber diameter

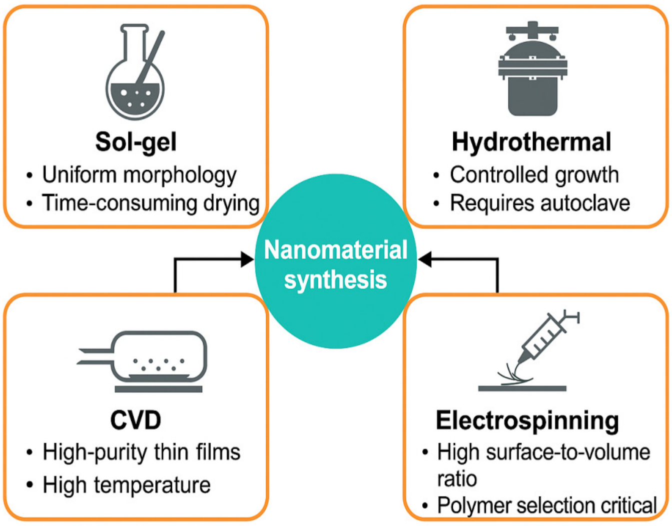

Fig. 6: Overview of Nanomaterial Synthesis Methods

energy applications as well as high power applications, Figure 7: Nanomaterials in Battery and Supercapacitor Architectures.

Batteries

In lithium ion, sodium ion and solid state battery, nanomaterials that have nanostructured architecture like metal oxides, graphene, and CNTs enhance better capacity retention, cycling stability and electrode electrolyte interface. It is hardier due to its quick ion diffusion and stronger mechanical integrity, mainly under extended cycling, owing to the high surface area and porosity tunability.

Supercapacitors

In electric double-layer capacitors (EDLCs) and metal oxides/conducting polymers in pseudocapacitors, carbon nanomaterials play a benefit. Nanostructuring helps achieve better charge storage due to short pathways of ions, high conductivity and hybrid functionality, and thus offers the best of both worlds in the charge storage capacity of batteries and the power storage capacity of capacitors.

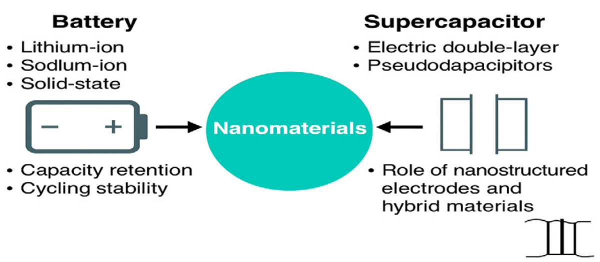

Fig. 7: Nanomaterials in Battery and Supercapacitor Architectures

Energy Conversion Applications

The functional nanomaterials are relevant in improving the efficiency of the energy conversion systems through the capability to facilitate a superior charge transport, catalysis, and thermal management.

Fuel Cells

N-doped carbons, TMDs, and MOF-derived carbons are being used as low-cost substitutes to Pt both in oxygen reduction and hydrogen oxidation reaction. Refined by large surface area and tuneable active sites, their electrochemical performance and durability is enhanced.

Photocatalysis and Solar Fuels

Water splitting and reduction of CO 2 are possible using photocatalysts such as perovskites, g -C 3 N 4 and TiO 2 based nanocomposites. Light absorption, charge separation and stability are improved by engineering the heterojunction and integrating co-catalysts as strategies.

Thermoelectrics

By nanostructuring thermoelectric materials (e.g., Bi 2 Te 3, PbTe) increases ZT values by eliminating phonon conduction without significantly reducing electrical conductivity. Nanocomposites and interface engineering will revolutionize the next generation thermal-to-electric conversion systems.

Challenges and Research Gaps

Although there are indications of functional nanomaterials, suitable for energy storage and conversion, there exist a number of obstacles to uptake into the real world (Table 2):

8. Future Perspectives

With the evolution of functional nanomaterials toward wide applications in energy storage and conversion, future research directions are targeting possible shortcomings to mend them and uncharted technological domains to explore. These direction are the ones that are likely to have a profound influence on the design of future high performance, sustainable and intelligent energy systems:

- Smart Hybrid Nanostructures: Self-healing, stimuli responsive and adaptive nanomaterials are going to be developed, which will increase the reliability and functionality in long-term use. Due to such response to environmental signals (temperature, pH or mechanical stress), those materials can be useful in autonomous systems,

Table 2: Summary of Key Challenges and Strategic Interventions in Nanomaterial-Based Energy Systems

Challenge	Description	Proposed Strategy
Stability	Nanomaterials often degrade under prolonged electrochemical, thermal, or photoactive conditions, compromising long-term device reliability.	Development of protective surface coatings, core-shell structures, and encapsulation strategies to improve durability.
Scalability	Many high-performance nanomaterials are synthesized using complex or costly lab-scale processes not suitable for mass production.	Adoption of low-cost, scalable methods such as spray pyrolysis, microwave-assisted synthesis, or green chemistry protocols.
Toxicity	The use of heavy metals (e.g., Pb in perovskites, Cd in quantum dots) raises concerns about environmental and biological safety.	Transition toward eco-friendly materials and implementation of lifecycle assessment (LCA) to evaluate environmental impact.
Interface Engineering	Inefficient charge transfer or recombination at material interfaces reduces device efficiency.	Use of engineered heterojunctions, interlayer modifications, and binder-free electrode architectures for enhanced interfacial performance.

as well as for hostile conditions.

- AI- Assisted Design: Artificial intelligence (AI) and machine learning (ML) are progressively incorporated into nanomaterials discovery and optimization process. Structure-property relationships are predictable and data-driven methods can speed the screening of candidate materials and provide synthesis parameters to help decrease the trial-and-error phase of data collection in experiments.
- Green Synthesis Strategies: A greater focus is being directed towards the utilization of eco-friendly, bio-mimicking, and low-energy-conversion production routes with minimal byproducts that are toxic and reduced energy use. Investigations are underway to devise and develop scalable, sustainable methods of manufacturing nanomaterials that include microwave-assisted synthesis, solvent-free processes and microbial use as assistance.
- Integrated System: Embedded energy generating devices such as nanogenerators, harvesters, and energy storage modules will be more flexible and stretchable that will be used in wearable form. The applications in next generation soft robotics, biomedical implants, and sensor networks based on the IoT will be supported through such systems.

Unitedly, these trends point to the transition to smart, sustainable and application-specific nanomaterials, which will bridge the gap between basic research and to-scale technological breakthroughs¤.

Conclusion

Nanomaterials are a cutting edge in the technological advancement and implementation of innovative energy storing and releasing technology. Their structurally tunable, electronic and interfacial properties allow significant increases in the energy density, charge transport and long term operational stability. Engineering of these materials to the nanoscale: via controlled morphology, hybridization and surface modification allows researchers to tune performance to suit application specific requirements across battery, supercapacitor, fuel cell and photocatalytic platforms.

Nevertheless, the conception of laboratory-based innovation needs to be translated into technologically feasible products, which still faces an uphill challenge in the areas of material scaling, environmental sustainability and integrating technologies. The next innovations will come as a result of interdisciplinary work between materials science, computational prediction, processing engineering, and data-driven optimization. Green synthesis, AI-assisted design, and application-based architectures will become key to making the task of creating multifunctional nanomaterials less an engineering feat but a sustainable one, both in the environmental sense and in economic terms.

After all, the multifunctionality of smart nanostructures, eco-friendly manufacturing, and system-wide engineering will define the future of next-generation energy systems that can achieve the 21 st century decarbonization and energy resilience goals on a global scale.

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